***Ab initio* methods**	Methods based on the local-density approximation model used to reveal locations of atomic nuclei at equilibrium as well as energies and spatial distribution of a material's electrons.
All-electron model	Model based on the local-density approximation used to calculate the motion of all electrons in a solid.
Atomistic	Of or relating to atoms. In modeling, atomistic simulations are concerned with length scales on the order of 10^{-8} to 10^{-9} m.
Constitutive relation	A tabulation of the behavior, such as the force required to stretch a certain distance, of a particular material that depends on its constitution or structure. The variety of behaviors of different materials, such as metals and glasses, enters continuum models through constitutive relations.
Continuum model	A model, useful for solving practical engineering problems, that treats an object or structure as a continuous material. Such models take into account, for example, regions of stress and strain, but they do not simulate the atomic structure of the system.
Ductile	Deformation of a material without fracture.
Elastic	Deformation of a material without permanent loss of size or shape.
Interstitial	In a crystalline material, atoms or ions that occupy spaces between other atoms or ions in the crystal lattice are called interstitial.
Local-density approximation model	Model used to determine the atomic and electronic structures of materials. These include crystal structure and density, internal atomic coordinates, structural phase transitions, and associated transition pressures.
LODTM	Large-optics diamond turning machine at LLNL.
Mesoscale simulation	A simulation concerned with the objects that define the microstructure of a material, such as dislocations and grain boundaries.
Model force laws	Laws used to approximate the forces among atoms. These laws are useful for larger-scale calculations, where *ab initio* methods would be too time consuming.
Molecular dynamics (MD) simulation	A modeling tool to study the statistical mechanical properties of a collection of atoms. In an MD calculation, atomic motion is simulated by solving Newton's equations of motion ($F = m \times a$) for a large collection of atoms.
Multilayers	Structures made of alternating layers of different materials, some as thin as 5 nm.
Nanotribology	The science of fundamental surface processes at the atomic scale, also known as molecular tribology. See tribology.

Plastic	A permanent change in shape or size when a material is subjected to a stress.
Polarization cloud	The region around a charged particle (when embedded in a gas of electrons) into which the electrons are either attracted or repelled.
Pseudopotential model	Method based on the local-density approximation used to calculate the motion of only the valence electrons in a solid.
Quasiparticle method	Method used to calculate the self energy of an excitation by including the effects of the polarization cloud. The complete excitation—an added electron or hole plus its polarization cloud—is called a "quasiparticle."
Relaxed surface	A material surface in which the atoms are at equilibrium.
Scintillator	A material that emits flashes of light in response to ionizing radiation. Such materials are used to identify brief showers of secondary particles, monitor radiation doses, and identify environmentally threatening sources.
Self energy	The reduction in energy of an electron or hole as other electrons move away from it.
Tribology	The science of interacting surfaces in relative motion, namely friction, lubrication, wear, and adhesion.
Valence electrons	Those electrons active in the chemical bonding of materials.